

4-(Chloromethyl)-2-ethoxy-1,3,2lambda⁵-dioxaphospholan-2-one

67554-11-4 | DTXSID50791173

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 5.80

Global applicability domain: Inside

Local applicability domain index: 9.72e-01

Confidence level: 8.38e-01

Nearest Neighbors from the Training Set

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1-Chloronaphthalene

Measured: 5.80

Predicted: 5.80

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2-Chloronaphthalene

Measured: 5.80

Predicted: 5.80

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Biphenyl

Measured: 6.15

Predicted: 5.83

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1,2,4,5-Tetrachlorobenzene

Measured: 5.63

Predicted: 5.67

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1,2,3,5-Tetrachlorobenzene

Measured: 5.55

Predicted: 5.67